Russian Journal of General Chemistry 2003 vol.73 N6, pages 921-927

Quantum-chemical estimation of the stability and reactivity of diphosphonium salts

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Abstract

For a series of diphosphonium salts containing two positively charged covalently bonded phosphorus atoms, XnY3-nP +P+XnY3-n (X = alkyl substituent, Y = amino group, n = 0-3), the stability, reactivity, and P-P bond strength were evaluated by various physicochemical methods. The P-P bond energy is appreciably influenced by both steric factors and donor properties of the substituents. The calculations confirmed that transformations of diphosphonium salts can involve cleavage of both P-P and P-N (or P-C) bonds.

http://dx.doi.org/10.1023/A:1026304918818